

Modeling the Fate of Synthetic Pyrethroids Permethrin, Deltamethrin, Bifenthrin, Cyfluthrin, Lambda-cyhalothrin, Cypermethrin, Esfenvalerate, and Fenpropathrin through a Large Scale Wastewater Treatment Plant in Suffern, New York

Report: Cleary, J.G. and McGrath, J. 2009. Modeling the Fate of Pyrethroids through Suffern, NY Wastewater Treatment Plant. Unpublished study performed by HDRHydroQual, Inc, Mahwah, N.J. and submitted by the Pyrethroid Working Group, Greensboro, N.C. HDRHydroQual Project Identification PYWG.001.002. December 2009. (MRID 48072901.)

Document No.: MRID **48072901**

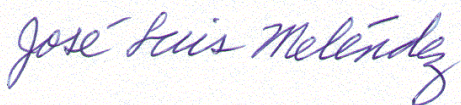
Guideline: Not applicable, this is a non-guideline study.

Statements: The study WAS NOT conducted in compliance with Good Laboratory Practice Standards (GLPS) set forth in Title 40, Part 160 of the Code of Federal Regulations (p. 3). The authors indicate that GLP standards do not apply to this document (p. 3). Signed and dated Data Confidentiality was provided (p. 2). Quality Assurance, and Authenticity Certification statements WERE NOT provided. A signatures page was provided (p. 4).

Classification: This study is considered **supplemental**. A major discrepancy was observed in the predicted distribution of pyrethroids in various compartments between the current New York and a concurrently reviewed study involving a plant in California (MRID 48857505). Compared to the CA study, this study was more limited in scope with fewer samples taken and analyzed. The study was not conducted in compliance with Good Laboratory Practice (GLP) Standards. Certain permethrin results were omitted from the summary results tables.

PC Codes	Permethrin	109701¹
	Bifenthrin	128825
	Cyfluthrin	128831
	Lambda-cyhalothrin	128897
	Cypermethrin	109702
	Deltamethrin	097805
	Esfenvalerate	109303
	Fenpropathrin	127901

Signature:



Reviewer:

José Meléndez, EPA

August 19, 2014

Signature:



Reviewer:

Stephen P. Wente, EPA

August 19, 2014

¹ This study will be filed in EFED in the folder for PC code 109701.

Executive Summary

In a non-GLP study, the software TOXCHEM+ was used to estimate the fate of eight pyrethroids in a treatment plant. The software is configured according to the plant's treatment train, and estimates dissolved and total concentrations of a chemical in the effluent of each unit process. It accounts for mechanisms such as stripping and volatilization, sorption, and aerobic and anaerobic degradation. The fate of organic contaminants in wastewater (*e.g.*, synthetic pyrethroid insecticides), can be predicted using a mass balance and transfer approach in which fate mechanisms compete with each other. When one mechanism increases (*e.g.*, sorption), another should decrease (*e.g.*, volatilization). The Village of Suffern Sewage Treatment Plant (Suffern, New York) was modelled in this study. Seven wastewater and five biosolid samples were obtained, during a period of no heavy rain and no plant upsets. Suspended solids in wastewater and total solids in biosolid samples, were measured. Samples were also analysed for pyrethroids. Each unit process (*i.e.*, each treatment process of the plant) was calibrated using flow and solids concentrations monitoring results.

Important physiochemical and fate characteristics needed to determine the fate of pyrethroids in the treatment plant were the octanol/water partition coefficient (*Log K_{OW}*), the Henry's Law Coefficient (both were taken from the open literature, Laskowski 2002), and the aerobic biodegradation rate. The aerobic biodegradation rate was initially set at the same default value for all pyrethroids, and each chemical's density was established at a set value of 1.0 g/mL. The anaerobic biodegradation was assumed to be negligible. Based upon the individual properties of each pyrethroid, with the exception of bifenthrin, it was expected that they would predominantly bind to solids. However for bifenthrin, which has a higher Henry's Law Coefficient, it was expected that a higher fraction of the chemical would be transferred to the atmosphere.

After configuring the plant and entering the physiochemical and fate characteristics of the pyrethroids, the aerobic biodegradation rate coefficients were calibrated, with pyrethroid concentrations, except for deltamethrin, which was too low to allow for calibration. **Table 1** provides a synopsis of the results. Opposed to a SRCSD study reviewed concurrently, in this study it was predicted that sorption is the main removal pathway for pyrethroids, followed by biodegradation. Based on a sensitivity analysis, with a variation of the Henry's Law coefficient (due to various reported solubility values in the open literature), for bifenthrin emissions would range from 19.5 to 24.5% of the applied mass.

Table 1. Results Synopsis: Predicted Distribution of Pyrethroids in a POTW in Suffern, NY

Chemical	Influent (g/day) ¹	Sludge (%)	Biodegraded (%)	Emitted (%)	Effluent (%)
Bifenthrin	0.28	64.65	9.28	24.45	1.62
Cyfluthrin (α,β) ²	0.31	62.84	31.82	0.42	4.91
Cypermethrin (α,β) ²	1.91	67.38	29.24	0.02	3.36
Deltamethrin	Not calculated ³	35.97	57.67	0.06	6.30
Esfenvalerate	0.05	58.13	36.84	0.02	5.00
Fenpropathrin	0.04	62.45	34.39	0.05	3.11
<i>Lambda</i> -cyhalothrin	0.04	75.78	13.95	0.02	10.25
Permethrin	3.93	62.61	36.08	0.05	1.26

Data was taken from Table 6, page 35 of the study report, and Table 7, page 36 of report. All percentages were reported to two decimal values in the report.

¹ Results from calibration in TOXCHEM+.

² The *alpha*- and *beta*-isomers had very similar properties and were taken together.

³ For deltamethrin the concentrations were too low to allow for recalibration of the default biodegradation rate coefficient.

I. Material and Methods

A. Materials: For structures of the test substances, see **Attachment 1**. The test materials were not radiolabeled. Batch numbers were not provided.

Table 2. Test Materials¹

Applicant's Code Name	PC Code	Chemical Name	Purity (%) ²
Bifenthrin	128825	(2-Methyl[1,1'-biphenyl]-3-yl)methyl 1 3-(-2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethylcyclopropane carboxylate	NR
Cyfluthrin	128831	Cyano(4-fluoro-3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate	NR
α -Cyfluthrin	N/A	Refer to Attachment 1. ⁴	NR
β -Cyfluthrin	118831	Refer to Attachment 1. ⁴	NR
<i>Lambda</i> -cyhalothrin	128897	[1a(S*),3a(Z)]-(\pm)-cyano(3-phenoxyphenyl)methyl 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl cyclopropanecarboxylate	NR
Cypermethrin	109702	(+/-)-a-cyano (3-phenoxyphenyl) methyl (+/-) cis. trans- 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropane carboxylate	NR
α -Cypermethrin	209600	Refer to Attachment 1. ⁴	NR
β -Cypermethrin	N/A	Refer to Attachment 1. ⁴	NR
Deltamethrin	097805	(S)-Cyano(3-phenoxyphenyl)methyl(1R,3R)-3-(2,2-dibromoethenyl)-2,2-dimethylcyclopropanecarboxylate	NR
Esfenvalerate	109303	((S)-Cyano(3-phenoxyphenyl)methyl(S)-4-chloro-a/p/7a-(1-methylethyl)benzeneacetate)	NR
Fenpropathrin	129701	Alpha-cyano-3-phenoxybenzyl-2,2,3,3-tetramethylcyclopropane carboxylate	NR
Permethrin	109701 ³	(3-Phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate	NR

¹ Refer also to **Attachment I** for structures and CAS numbers of these compounds.

² NR=not reported.

³ This DER will be filed under PC Code **109701** in the EFED file room.

⁴ The *alpha*- and *beta*-isomers were modeled together since they exhibited and are expected to behave similarly.

B. Wastewater Treatment Plant: The study involved the Village of Suffern Sewage Treatment Plant (Suffern, NY), which is a plant receiving discharges from a pharmaceutical manufacturer and a hospital, with a low average flow of 1.9 million gallons per day (MGD), compared to the CA treatment plant. This treatment plant includes the following treatment processes: primary clarification, trickling filtration with secondary clarification, activated sludge with integral clarification, disinfection through ultraviolet light, and sludge from all three clarification systems is processed in an anaerobic digester, dewatered through centrifugation, and transferred off site.

C. Study Design: Hydromantis, Inc. performed the model configuration of each process occurring in the treatment plant using the software TOXCHEM+. Firstly, information about the treatment plant was gathered including design, specifications, hydraulics data, operation manuals, information from the treatment plant personnel, as well as other data about the plant, such as plant flows, tank volumes, operating conditions, *etc.*, to simulate the treatment train. In Suffern, seven wastewater and five biosolid samples were taken, during a period of no heavy rain and no plant upsets. Suspended solids in wastewater, and total solids in biosolid samples, were measured. Chemical oxygen demand (COD) was measured for total and filtered (0.45 μm filter) wastewater samples. Total organic carbon (TOC) and dissolved organic carbon (DOC) were measured for total and filtered plant influent and effluent. The solids mass balance of the treatment plant was particularly necessary, given that pyrethroids are expected to bind to solids. Samples were also gathered for pyrethroid analysis. Each unit process (*i.e.*, each treatment process of the plant) was calibrated using flow and solids concentrations monitoring results.

D. Modeling Effort: Once the treatment plant was configured, the modeling of eight pyrethroids was performed. Important physiochemical and fate characteristics needed to determine the fate of pyrethroids in a treatment plant were the octanol/water partition coefficient ($\text{Log } K_{\text{OW}}$), the Henry's Law Coefficient, and the aerobic biodegradation rate. The anaerobic biodegradation was assumed to be negligible, while the volatilization (Henry's Law Coefficient) and sorption ($\text{Log } K_{\text{OW}}$) properties were taken from Laskowski (2002). The aerobic biodegradation was initially set at the same default value for all pyrethroids, and each chemical's density was established at a set value of 1.0 g/mL. Based upon these properties, with the exception of bifenthrin, it was expected that pyrethroids would predominantly bind to solids. For bifenthrin, which has a higher Henry's Law Coefficient, it was expected that a higher fraction of the chemical would be transferred to the atmosphere.

II. Results and Discussion

A. Results of QA/QC Samples

- 1. Samples:** Solids, secondary clarifier sludge, and water samples (one replicate each), were taken for QA/QC analysis for each of 10 pyrethroids. All analyses were conducted by GC/MS-NCI methodology (not further described). Blank solids and blank water were conducted and reported (one replicate each). For each type of sample spikes were also reported, in duplicate analyses. Analyses results for each of *alpha*-cyfluthrin, *beta*-cyfluthrin, *alpha*-cypermethrin, and *beta*-cypermethrin were reported [note that in the modeling effort using TOXCHEM+, the *alpha*- and *beta*-isomers of cyfluthrin and cypermethrin were combined].
- 2. Blank Solids:** Blank solids results were reported as <10 ng/g dw for all 10 pyrethroids. Blank solids recoveries ranged from 90 to 106% recovered (spiking level not reported) (Table A-4 of Appendix 1, page 27).
- 3. Secondary Clarifier Sludge:** Results of the secondary clarifier sludge ranged from <10 to 1140 ng/g dw (Table A-3, Appendix 1, page 25). The higher value in the range

belongs to permethrin. Recovery results for the secondary clarifier sludge spike (spiking level not reported), ranged from 87 to 186% recovered (Table A-4 of Appendix 1, page 27). The higher recoveries may be due to the presence of pyrethroids in background levels; however, the spiking level was not reported and no further information was provided and this cannot be confirmed.

4. **Blank Water:** Laboratory blank water was reported as <10 ng/L for all pyrethroids. Recoveries for these samples ranged from 75 to 113% recovered (Table A-4 of Appendix 1, page 27).

B. Findings

5. **POTW Pyrethroid Calibration in TOXCHEM+:** In this study, the biodegradation rate coefficients were calibrated, with pyrethroid concentrations, except for deltamethrin, which was too low to allow for calibration. **Table 3** provides a summary of the pyrethroid input values used in the model. For all chemicals, the density was set to 1.0 g/mL. Furthermore, the aerobic biodegradation rate coefficient was initially set to 0.001 L/mg VSS-h and then calibrated. Values in the table are the results after calibration. It was noted that the calibrated aerobic biodegradation rates were similar to the initially set value of 0.001 L/mg VSS-h.

Table 3. Pyrethroid Properties Used in Modeling the Suffern, NY POTW in TOXCHEM+

Chemical\Property	Molecular Weight (g/mole)	Density (g/mL) ¹	Henry's Law Coefficient (L _{liq} /L _{gas})	Log Kow	Calibrated Aerobic Biodegradation Rate Coefficient (L/mg VSS-h)
Bifenthrin	422.9	1.0	0.294	6.4	0.001
Cyfluthrin (α,β) ²	434.3	1.0	1.51×10^{-4}	5.97	0.001
Cypermethrin (α,β) ²	416.3	1.0	1.39×10^{-6}	6.54	0.0018
Deltamethrin	505.2	1.0	1.27×10^{-5}	4.53	0.001
Esfenvalerate	419.9	1.0	5.73×10^{-6}	5.62	0.001
Fenpropathrin	349.4	1.0	2.58×10^{-5}	6.0	0.0017
Lambda-cyhalothrin	449.9	1.0	7.77×10^{-6}	7.0	0.0004
Permethrin ³	391.3	Not reported	Not reported	Not reported	Not reported

Data obtained from Table 3 of Appendix 2, page 32 of study report.

¹ Density was set the same set value for all pyrethroids.

² The *alpha*- and *beta*-isomers had very similar properties and were taken together, despite them being analysed separately.

³ Data for permethrin was missing from Table 3 of Appendix 2 (page 32) or Table 2 (page 15) of study report.

6. **Measured vs. Predicted Concentrations in Effluent and Sludge:** **Table 4** summarizes the measured and predicted concentrations in filtered and total effluent waters, and sludge cake. Since the measured filtered effluent waters were reported as <10 ng/L, all the predicted values were within this range. The measured and predicted total effluent water concentrations were within the same order of magnitude of each other. The sludge cake measured concentrations were in a range of 4300 to 567000 ng/L. The predicted sludge cake concentrations were also within the same order of magnitude than the measured concentrations.

Table 4. Measured and Predicted Concentrations in Effluent (Filtered & Total) and Sludge

Chemical\Conc. (ng/L)	Measured Filtered Effluent	Predicted Filtered Effluent	Measured Total Effluent	Predicted Total Effluent	Measured Sludge Cake	Predicted Sludge Cake
Bifenthrin	<10	0.371	<10	0.628	103100	40580
Cyfluthrin (α,β) ¹	<10	1.50	1.88	2.09	55830	43320
Cypermethrin (α,β) ¹	<10	2.76	9.5	5.08	249100	286600
Deltamethrin	Not reported					
Esfenvalerate	<10	3.0	<10	10.5	6560	5940
Fenpropathrin	<10	0.137	<10	0.193	4310	6280
<i>Lambda</i> -cyhalothrin	<10	0.23	0.54	0.58	10030	7010
Permethrin	<10	4.7	<10	6.9	567000	555000

Data was taken from **Table 5** page 34 of study report.

¹ The *alpha*- and *beta*-isomers had very similar properties and were taken together, despite them being analysed separately.

- 7. Predicted Compartment Distributions:** The predicted distribution in different compartments of the Suffern, NY is shown in **Tables 1** (p. 2, reported as a percentage) and **Table 5** (reported in grams/day). According to the modeling results, the major portion of each and all the synthetic pyrethroids was expected to occur in sludge, followed by biodegradation. (In contrast, in the CA study it was predicted that biodegradation is the main removal pathway for pyrethroids, followed by sorption.) Only bifenthrin was predicted to be emitted to air to a relatively high degree (~24%).

Table 5. Predicted Distribution of Synthetic Pyrethroids in Suffern, NY POTW

Chemical	Influent (g/day)	Sludge (g/day)	Biodegraded (g/day)	Emitted to Air (g/day)	Effluent (g/day)
Bifenthrin	0.28	0.18	0.03	0.07	0.005
Cyfluthrin (α,β) ¹	0.31	0.19	0.1	0.001	0.02
Cypermethrin (α,β) ¹	1.91	1.29	0.56	3.98x10 ⁻⁴	0.06
Deltamethrin	Not calculated ²				
Esfenvalerate	0.05	0.03	0.02	8.64x10 ⁻⁶	0.002
Fenpropathrin	0.04	0.03	0.02	2.2x10 ⁻⁵	0.001
<i>Lambda</i> -cyhalothrin	0.04	0.03	0.006	9.52x10 ⁻⁶	0.004
Permethrin	3.93	2.46	1.42	0.002	0.05
Total Pyrethroid	6.56	4.21	2.15	0.07	0.14

Data was taken from Table 7 of Appendix 2, page 36 of the study report.

¹ The *alpha*- and *beta*-isomers had very similar properties and were taken together, despite them being analysed separately.

² For deltamethrin the concentrations were too low to allow for recalibration of the default biodegradation rate coefficient.

- 8. Sensitivity Analysis:** Based on a sensitivity analysis, with a variation of the Henry's Law coefficient (due to a wide range of open literature-reported solubility values), for bifenthrin emissions would range from 19.5 to 24.5% of the applied mass. An additional sensitivity analysis was conducted with deltamethrin, with variation of the *Log K_{ow}*. The main effect was on the level of sorption to solids, with the level of biodegradation being the other variable affected. The emissions to the atmosphere saw very little variation.

III. Study Deficiencies and Reviewer's Comments

- A.** An important discrepancy was observed in the predicted distribution of pyrethroids in various compartments between the current NY and a concurrently reviewed study involving a plant in CA. According to the modeling results, the major portion of each and all the synthetic pyrethroids was expected to occur in sludge, followed by biodegradation. (In contrast, in the CA study it was predicted that biodegradation is the main removal pathway for pyrethroids, followed by sorption.)
- B.** The study was not conducted in compliance with Good Laboratory Practice Standards set forth in Title 40, Part 160 of the Code of Federal Regulations (p. 3 of the study report). The study does not provide any indications as to which were the main procedures that departed substantially from GLPs.

IV. Comparison of Studies Reviewed Concurrently

A major complicating factor for interpreting the studies of pyrethroid fate in publically-owned treatment works (POTWs) is understanding the uncertainty inherent in the mass balances presented in these studies. Two of these studies, MRID 48072901 and MRID 48857505, model the fate of pyrethroids in POTWs in New York (denoted POTW NY) and California (POTW CA), and the third study (MRID 48762906) is a bench scale laboratory model of the POTW treatment processes and influent from POTW NY (denoted Lab NY). The basic mass balance follows a parcel of water through real POTWs (POTW CA and NY) or a simulated POTW (Lab NY) from plant influent concentration to plant effluent concentration both of which are measured and therefore, relatively certain values. As the parcel of water moves through the POTW, pyrethroids are lost from the water parcel due to partitioning to solids or sludge, metabolism, and volatilization.

The concentration of pyrethroids in sludge is another measured value; however the uncertainty associated with these measured values should increase with increasing solids in the medium measured. Pyrethroids tend to bind to the organic material in the solids. Because all of these POTW studies used non-radiolabeled pyrethroids, it is likely that a significant fraction of the pyrethroid residues were not extracted in those samples with a lot of solids. For example, radiolabeled alpha-cypermethrin aerobic aquatic metabolism studies (MRID 48425011 and 48425012) found un-extracted residues in excess of 40% of applied radioactivity. Therefore, the effluent concentration (very little solids) is more certain than the influent concentration (more solids), which is more certain than the sludge concentration.

The amount of pyrethroids volatilized is based on the Henry's Law Constant of each pyrethroid and the amount time spent undergoing aerobic biological treatment in each facility. However, it would also be decreased by how much partitioning to solids and biodegradation had already

occurred within the POTW. Therefore, if the actual sludge concentration was higher (due to un-extracted residues) than measured, the amount volatilized should be lower.

Biodegradation was estimated from the difference between the measured influent and the measured effluent, measured sludge, and estimated volatilization (biodegradation = influent – sum [effluent, sludge, and volatilization]). Therefore again, if the actual sludge concentration was higher (due to un-extracted residues) than measured, the amount of pyrethroids biodegraded should be lower. Based upon the dependence on the sludge measurement and the way this value is calculated, the biodegradation value should probably be treated as the least certain value reported.

In order to compare the three studies investigating the fate of pyrethroids in POTWs, an attempt was made to summarize the generalized mass balance produced by each study (**Table 6**). The POTW NY values are based on Table 7 of Appendix 2 (page 36 of the study report) after converting to percent of influent. The Lab NY values are from Table 9 of page 35 of the study report. Because the primary settling portion of the lab study did not work, only values from the aeration system were used for this comparison. The POTW CA values are from Table 12 on page 12 and Table 13 on page 13 of Attachment 1 of the study report (values are medians of three calibrations and may not add to 100%).

Table 6. Comparison of Pyrethroid Mass Balances within POTW across Studies.

Chemical	Study	Sludge (%)	Biodegraded (%)	Emitted (%)	Effluent (%)
Bifenthrin	POTW NY	64.29	10.71	25.00	1.79
	Lab NY	10.5	41.4	NE	48.1
	POTW CA	41.75	44.01	1.79	9.99
Cyfluthrin (α,β) ¹	POTW NY	61.29	32.26	0.32	6.45
	Lab NY	5.8	67.4	NE	26.8
	POTW CA	37.4	58.84	0.01	7.25
Cypermethrin (α,β) ¹	POTW NY	67.54	29.32	0.02	3.14
	Lab NY	5.4	70.8	NE	23.7
	POTW CA	29.85	65.21	<0.01	4.84
Deltamethrin	POTW NY	Not Measured in NY POTW			
	Lab NY	9.6	49.5	NE	40.9
	POTW CA	Not Measured in CA POTW			
Esfenvalerate	POTW NY	60.00	40.00	0.02	4.00
	Lab NY	12.5	43.6	NE	43.9
	POTW CA	Not Measured in CA POTW			
Fenpropathrin	POTW NY	75.00	50.00	0.06	2.50
	Lab NY	4.4	75.7	NE	19.9
	POTW CA	Not Measured in CA POTW			
<i>Lambda</i> -cyhalothrin	POTW NY	75.00	15.00	0.02	10.00
	Lab NY	14.4	34.2	NE	51.4
	POTW CA	42.04	50.68	<0.01	8.23
Permethrin	POTW NY	62.60	36.13	0.05	1.27
	Lab NY	5.1	81.6	NE	13.4
	POTW CA	33.38	63.75	<0.01	5.16

NE = Not Estimated

Comparing the percentage of the influent pyrethroids in the effluent (effluent values expected to be relatively certain due to low solids concentrations), it is clear that the Lab NY values do not align with the POTW NY and CA values. As explained in Lab NY report, the pyrethroids did not settle out with solids in the primary settling portion of the experiment, which appears to have allowed the pyrethroids attached to dissolved organic to carbon to resist biodegradation. Potentially, the Lab NY values are more representative of an overloaded or poorly functioning POTW.

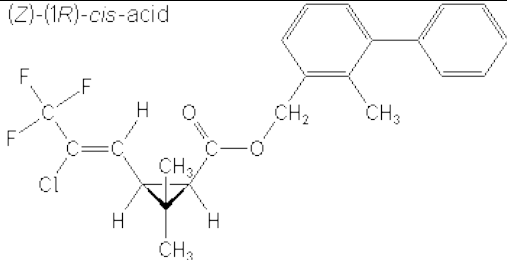
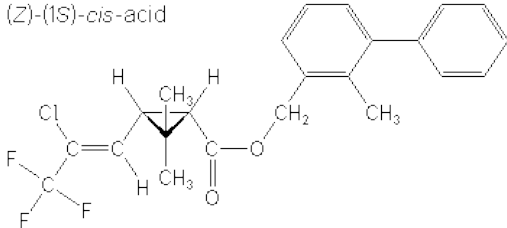
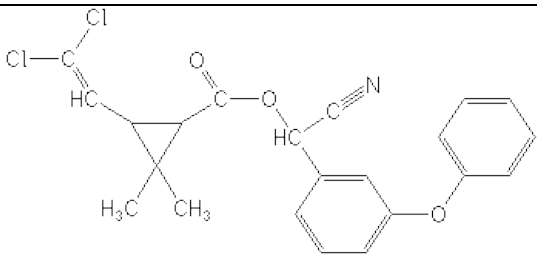
Comparing the POTW NY and CA effluent values yields relatively good agreement for those pyrethroids that can be compared (bifenthrin: 1.79 vs 9.99%; cyfluthrin: 6.45 vs 7.25%; cypermethrin: 3.14 vs 4.84%; *lambda*-cyhalothrin: 10 vs 8.23%; and permethrin: 1.27 vs 5.16%) considering that the values come from different POTWs with differing waste streams. Notice that if the somewhat uncertain influent values were higher due to un-extracted pyrethroid residues, the effluent percentages would be lower.

Other than the effluent values, the sludge values are the next most useful values from these studies for pyrethroid risk assessment. Considering the potential for un-extracted residues, the listed sludge percentages should probably be considered minimum values (i.e., the percentages of influent pyrethroids in biosolids are at least the values given in Table 1, but could be substantially higher).

V. References

Laskowski, D. 2002. Physical and Chemical Properties of Pyrethroids. Rev. Environ. Contam. Toxicol. 174:49-170.

Attachment 1: Chemical Names and Structures**TABLE 1.1. Test Compounds Nomenclature²**

Common name	Bifenthrin
IUPAC name	2-Methylbiphenyl-3-ylmethyl (Z)-(1R,3RS)-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylate.
CAS Name	(2-Methyl [1,1'-biphenyl]-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylate.
CAS #	82657-04-3.
Structure	<p>(Z)-(1R)-cis-acid</p>  <p>(Z)-(1S)-cis-acid</p> 
Common name	Cypermethrin.
IUPAC name	(RS)- α -Cyano-3-phenoxybenzyl (1R,3RS;1R,3SR)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate.
CAS Name	Cyano (3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate.
CAS #	52315-07-8.
Structure	
Common name	α-Cypermethrin
IUPAC name	Racemate comprising (R)- α -cyano-3-phenoxybenzyl (1S,3S)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate and (S)- α -cyano-3-phenoxybenzyl (1R,3R)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate
CAS Name	(R)-cyano(3-phenoxyphenyl)methyl (1S,3S)-rel-3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate
CAS #	67375-30-8

² Structures were obtained at http://www.alanwood.net/pesticides/index_cn_frame.html (accessed 03/20/14).

TABLE 1.1. Test Compounds Nomenclature²

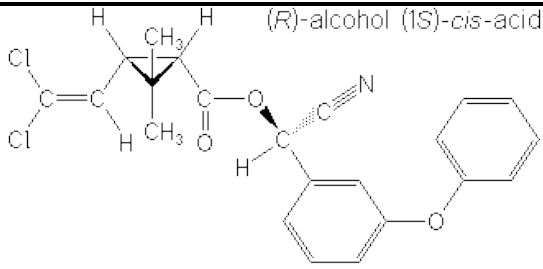
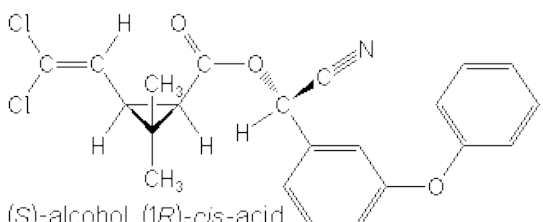
Structure	 
Common name	β-Cypermethrin
IUPAC name	Reaction mixture comprising the enantiomeric pair (<i>R</i>)-α-cyano-3-phenoxybenzyl (1 <i>S</i> ,3 <i>S</i>)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate and (<i>S</i>)-α-cyano-3-phenoxybenzyl (1 <i>R</i> ,3 <i>R</i>)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate in ratio approximately 2:3 with the enantiomeric pair (<i>R</i>)-α-cyano-3-phenoxybenzyl (1 <i>S</i> ,3 <i>R</i>)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate and (<i>S</i>)-α-cyano-3-phenoxybenzyl (1 <i>R</i> ,3 <i>S</i>)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate
CAS Name	Cyano(3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate
CAS #	65731-84-2

TABLE 1.1. Test Compounds Nomenclature²

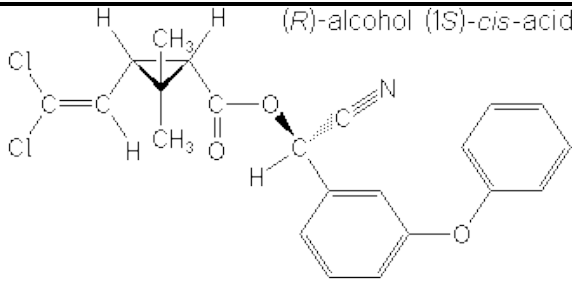
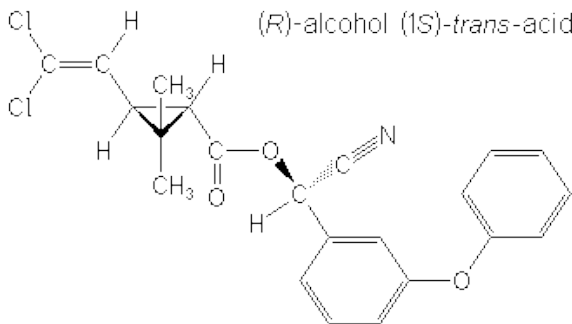
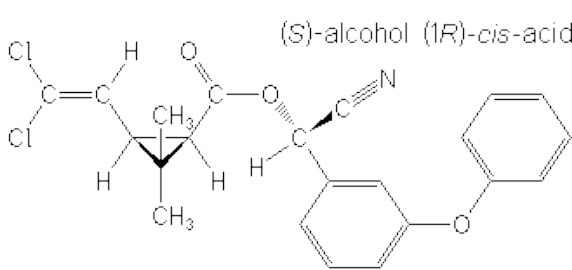
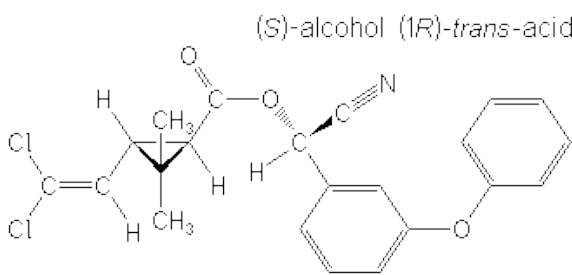
Structure	<p>(R)-alcohol (1S)-cis-acid</p>  <p>(R)-alcohol (1S)-trans-acid</p>  <p>(S)-alcohol (1R)-cis-acid</p>  <p>(S)-alcohol (1R)-trans-acid</p> 
Common name	Cyfluthrin.
IUPAC name	(RS)- α -Cyano-4-fluoro-3-phenoxybenzyl (1RS,3RS;1RS,3SR)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane carboxylate.
CAS Name	Cyano (4-fluoro-3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate.
CAS #	68359-37-5.

TABLE 1.1. Test Compounds Nomenclature²

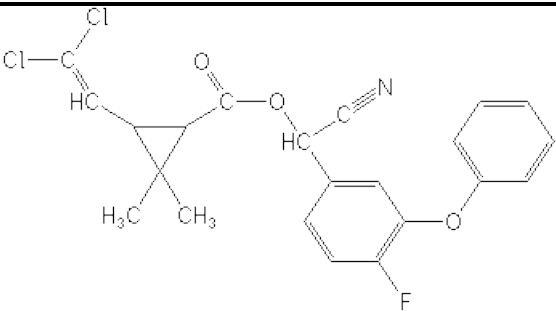
Structure	
Common name	<i>α</i>-Cyfluthrin
IUPAC name	Not available
CAS Name	Not available
CAS #	Not available
Structure	Not available
Common name	<i>β</i>-Cyfluthrin
IUPAC name	Reaction mixture comprising the enantiomeric pair (<i>R</i>)- <i>α</i> -cyano-4-fluoro-3-phenoxybenzyl (1 <i>S</i> ,3 <i>S</i>)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate and (<i>S</i>)- <i>α</i> -cyano-4-fluoro-3-phenoxybenzyl (1 <i>R</i> ,3 <i>R</i>)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate in ratio 1:2 with the enantiomeric pair (<i>R</i>)- <i>α</i> -cyano-4-fluoro-3-phenoxybenzyl (1 <i>S</i> ,3 <i>R</i>)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate and (<i>S</i>)- <i>α</i> -cyano-4-fluoro-3-phenoxybenzyl (1 <i>R</i> ,3 <i>S</i>)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate
CAS Name	Cyano(4-fluoro-3-phenoxyphenyl)methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate
CAS #	68359-37-5

TABLE 1.1. Test Compounds Nomenclature²

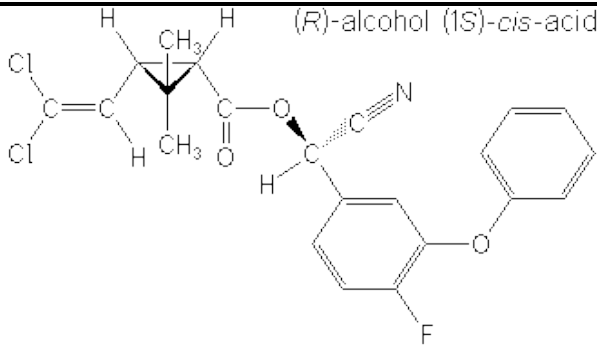
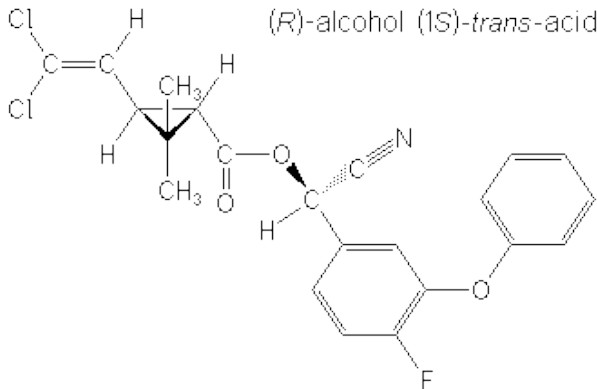
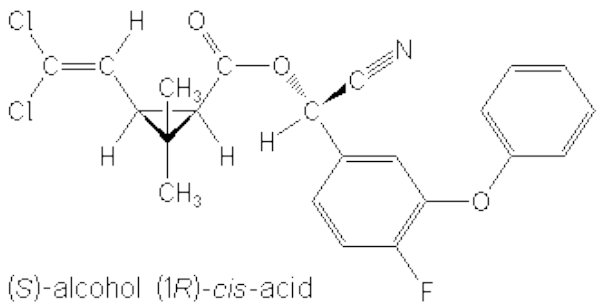
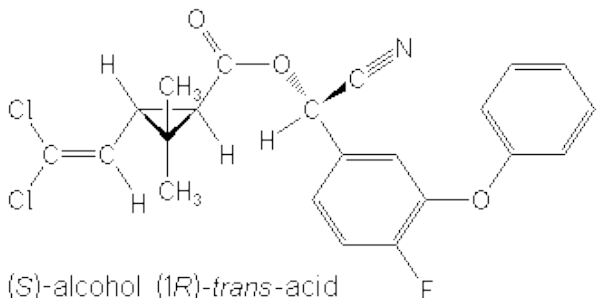
Structure	 <p>(R)-alcohol (1S)-cis-acid</p>  <p>(R)-alcohol (1S)-trans-acid</p>  <p>(S)-alcohol (1R)-cis-acid</p>  <p>(S)-alcohol (1R)-trans-acid</p>
Common name	Deltamethrin.
IUPAC name	(S)- α -Cyano-3-phenoxybenzyl (1R,3R)-3-(2,2-dibromovinyl)-2,2-dimethylcyclopropanecarboxylate.
CAS Name	1-[R-[1- α -(S*),3 α]]-Cyano(3-phenoxyphenyl)methyl 3-(2,2-dibromoethenyl)-2,2-dimethylcyclopropanecarboxylate.
CAS #	52918-63-5.

TABLE 1.1. Test Compounds Nomenclature²

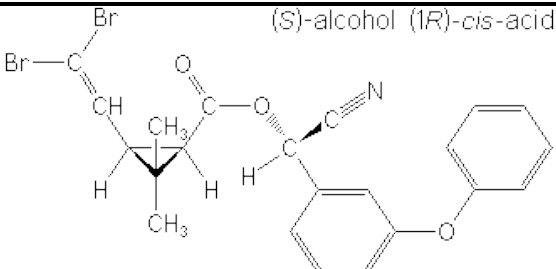
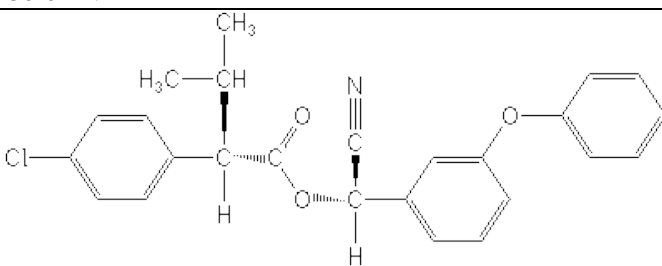
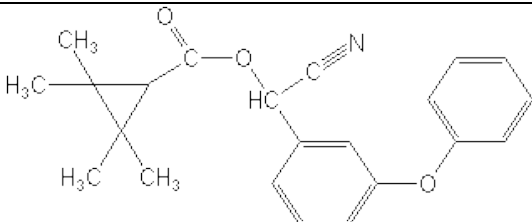
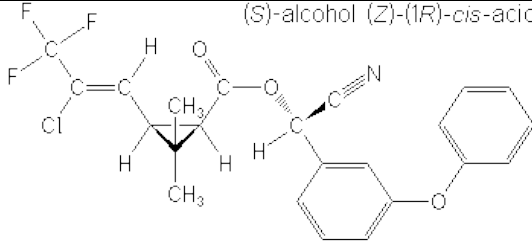
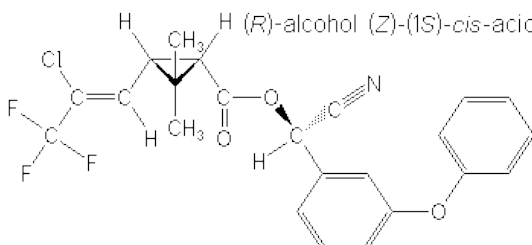
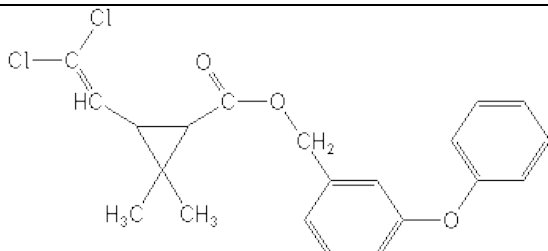
Structure	 <p>(S)-alcohol (1R)-cis-acid</p>
Common name	Esfenvalerate.
IUPAC name	(S)-α-Cyano-3-phenoxybenzyl (S)-2-(4-chlorophenyl)-3-methylbutyrate.
CAS Name	[S-(R*,R*)]-Cyano (3-phenoxyphenyl)methyl 4-chloro-2-(1-methylethyl) benzeneacetate.
CAS #	66230-04-4.
Structure	
Common name	Fenprothrin.
IUPAC name	(RS)-α-Cyano-3-phenoxybenzyl 2,2,3,3-tetramethylcyclopropanecarboxylate.
CAS Name	Cyano (3-phenoxyphenyl) methyl 2,2,3,3-tetramethylcyclopropanecarboxylate.
CAS #	64257-84-7.
Structure	
Common name	Lambda-cyhalothrin.
IUPAC name	Reaction product of equal quantities of (S)- and (R)- α-cyano-3-phenoxybenzyl (Z)-(1R,3R)-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethylcyclopropanecarboxylate.
CAS Name	[1α(S*),3α(Z)]-(±)-Cyano(3-phenoxyphenyl)methyl 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethylcyclopropanecarboxylate.
CAS #	91465-08-6.

TABLE 1.1. Test Compounds Nomenclature²

Structure	<p>(S)-alcohol (Z)-(1R)-cis-acid</p>  <p>(R)-alcohol (Z)-(1S)-cis-acid</p> 
Common name	Permethrin.
IUPAC name	3-Phenoxybenzyl (1RS,3RS;1RS,3SR)-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate.
CAS Name	(3-Phenoxyphenyl) methyl 3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropanecarboxylate.
CAS #	52645-53-1.
Structure	

¹ Structures were obtained at http://www.alanwood.net/pesticides/index_cn_frame.html (accessed 03/20/14).